A Computer Program for Electron Probe Microanalysis in the Fields of Metallurgy and Geology

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A comprehensive computer program has been written which should prove useful to investigators in both the fields of metallurgy and geology. The program is flexible in both input and output and is relatively easy for an inexperienced person to use. It is written in the Fortran language and can be used in the time sharing mode which is now available in many laboratories. The program is built up of a large number of subroutines which can be easily changed as the user sees fit or as new correction schemes become available. At present the following corrections are incorporated; the absorption correction of Philibert-Duncumb[1,2] recently modified by Heinrich[3], the atomic number correction of Duncumb and Reed[4] and the fluorescence correction of Reed[5]. Both K and L X-radiations are considered and the program will operate in either of two modes; conversion of raw intensity data to composition using an iterative procedure or conversion of compositional data to expected X-ray intensities. For problems in geology involving oxides, calculations are made with oxygen considered as a matrix element. Specimens and complex standards each containing up to nine elements can be treated and several standards can be used for each element measured to check the consistency of the answer. Also characteristic lines of elements in a sample measured at different probe accelerating potentials can be handled.

The program is rather unique with respect to the method of data handling and ease of operation. All the critical data for a given element, such as X-ray wavelengths, fluorescent yields, atomic weights, absorption edge jump ratios and the necessary factors for the calculation of absorption coefficients from Heinrich[6] for that element are stored on cards. These data are then used as needed for the elements under consideration in each problem. The compositional data for each of the standards available to the probe user are also placed on cards to be used when needed. The input data which specifies the problem of interest then requires a minimum of information, for example the take-off angle, dead time for each spectrometer, operating voltage, calculation mode, and the elements which are measured on each spectrometer. Even this input data can be supplied in a non-rigid format.

The program determines internally whether a fluorescence correction is necessary and calculates the initial intensity ratios. An exhaustive print out of the various correction factors can be obtained if desired along with approximate error limits for each of the calculated data points

References

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